This dataset contains:

Analytical characterisation of the new ligand and complex salts (CHN microanalysis)

^{1}H and ^{13}C NMR spectra of the new ligands L^2-L^4, and of $[\{Fe(L^1)\}_4(\mu\text{-}L^1)_4][BF_4]_8$ (raw data and plotted spectra).

Electrospray mass spectra (plotted spectra).

X-ray Crystallographic data:

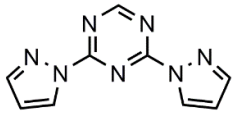
- Structure of L^2·MeCN (CCDC 1957574)
- Structure of L^4·2$CHCl_3$ (CCDC 1957573)
- Structure of α-L^7 (CCDC 1957575) and β-L^7 (not deposited with CCDC)
- Structure of $[\{Fe(L^1)\}_4(\mu\text{-}L^1)_4][BF_4]_8$·½$PzBF_3$·*n*MeCN (CCDC 1550948)
- Structure of $[Ag(\mu\text{-}L^2)]ClO_4$ (CCDC 1957577)
- Structure of $[Ag(NCMe)(\mu\text{-}L^2)]ClO_4$ (CCDC 1957576)
- Structure of $[Ag_4(\mu\text{-}L^3)_4][ClO_4]_4$ (CCDC 1957578)
- Structure of $[Ag_4(\mu\text{-}L^3)_4][ClO_4]_4$·3.2$MeNO_2$·1.2$H_2O$ (CCDC 1957579)
- Structure of $[Ag_4(\mu\text{-}L^3)_4][SbF_6]_4$·$MeNO_2$ (CCDC 1957580)
- Structure of $[Ag_4(\mu\text{-}L^4)_4][ClO_4]_4$·$MeNO_2$ (CCDC 1957581)
- Structure of $[Ag(NCMe)L^3]ClO_4$ (CCDC 1957582)
- Structure of $[Fe(NCS)_2(L^5)_2]$ (CCDC 1957583)
- Structure of $[Fe(NCS)_2(L^5)_2]$·MeOH (CCDC 1957584)
- Structure of $[Fe(NCSe)_2(L^5)_2]$·MeOH (CCDC 1957585)
- Structure of $[Fe(NCSe)_2(L^5)_2]$·½EtOH (CCDC 1957586)
- Structure of $[Fe(NCSe)_2(L^5)_2]$·½Me_2CO (CCDC 1957587)
- Structure of $[Fe(NCS)_2(\mu\text{-}L^6)]$ (CCDC 1957588)
- Structure of $[Fe(NCSe)_2(L^6)_2]$ (CCDC 1957589)
- Structure of $[Fe(NCS)_2(\mu\text{-}L^7)]$ (CCDC 1957590)
- Structure of $[Fe(NCSe)_2(\mu\text{-}L^7)]$ (CCDC 1957591)
- Structure of $[Fe(OH_2)_2(\mu\text{-}L^5)][ClO_4]_2$ (CCDC 1957592).

X-ray powder diffraction data (measured and simulated).

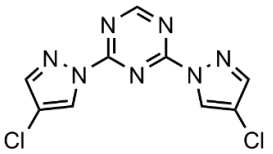
Solid state magnetic susceptibility measurements (raw and processed data).

Solution magnetic susceptibility measurements by Evans method (plotted NMR spectra and processed data).

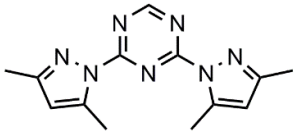
Ligands prepared during this study



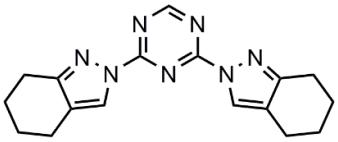
2,4-Di(pyrazol-1-yl)-6*H*-1,3,5-triazine
$C_9H_7N_7$
L^1



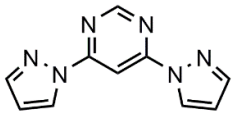
2,4-Di(4-chloropyrazol-1-yl)-6*H*-1,3,5-triazine
$C_9H_5Cl_2N_7$
L^2



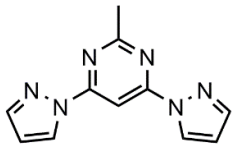
2,4-Di(3,5-dimethylpyrazol-1-yl)-6*H*-1,3,5-triazine
$C_{13}H_{15}N_7$
L^3



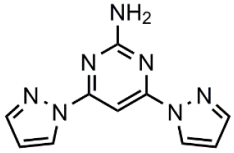
2,4-Di(4,5,6,7-tetrahydroindazol-2-yl)-6*H*-1,3,5-triazine
$C_{17}H_{19}N_7$
L^4



4,6-Di(pyrazol-1-yl)pyrimidine
$C_{10}H_8N_6$
L^5

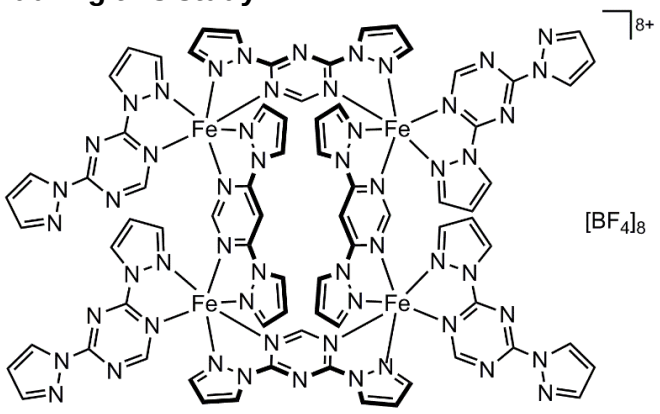


2-Methyl-4,6-di(pyrazol-1-yl)pyrimidine
$C_{11}H_{10}N_6$
L^6



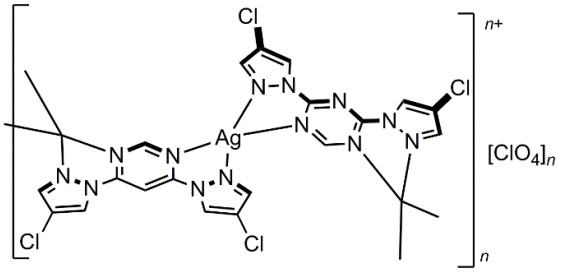
2-Amino-4,6-di(pyrazol-1-yl)pyrimidine
$C_{10}H_9N_7$
L^7

Complexes prepared during this study



Octakis-[2,4-di(pyrazol-1-yl)-6*H*-1,3,5-triazine]tetrairon(II) octa-tetrafluoroborate
$C_{72}H_{56}B_8F_{64}Fe_4N_{56}$
$[\{Fe(L^1)_4(\mu\text{-}L^1)_8][BF_4]_8$

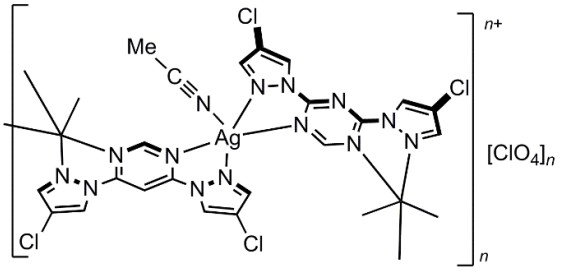
Complexes prepared during this study (continued)



catena-[2,4-di(4-chlorolpyrazol-1-yl)-6*H*-1,3,5-triazine]-silver(I) perchlorate

$C_9H_5AgCl_3N_7O_4$

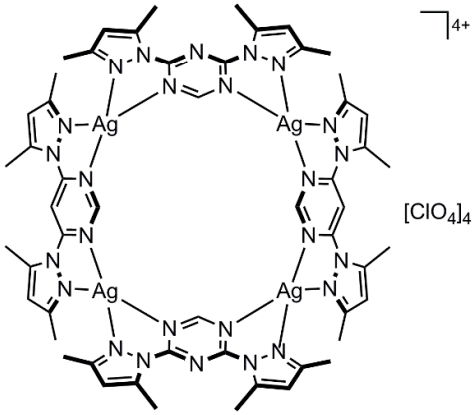
$[Ag(\mu\text{-}L^2)]ClO_4$



catena-[2,4-di(4-chlorolpyrazol-1-yl)-6*H*-1,3,5-triazine]-(acetonitrile)silver(I) perchlorate

$C_{11}H_8AgCl_3N_8O_4$

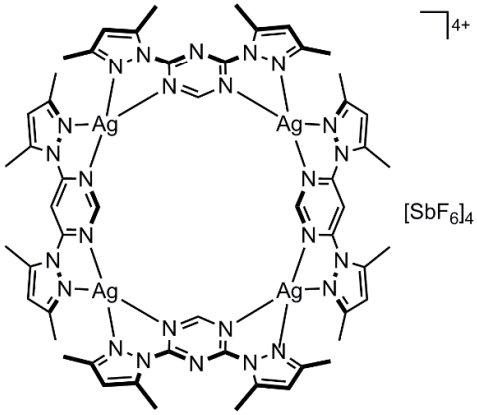
$[Ag(NCMe)(\mu\text{-}L^2)]ClO_4$



Tetrakis-[2,4-di(3,5-dimethylpyrazol-1-yl)-6*H*-1,3,5-triazine]-tetrasilver(I) tetraperchlorate

$C_{52}H_{60}Ag_4Cl_4N_{28}O_{16}$

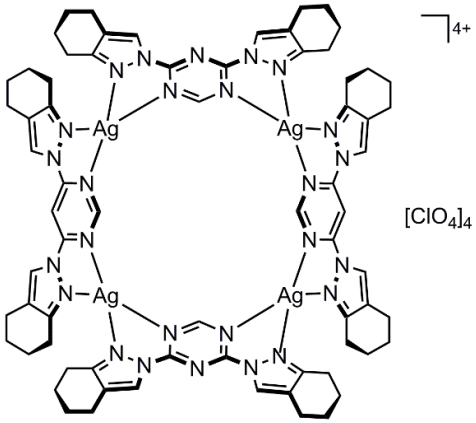
$[Ag_4(\mu\text{-}L^3)_4][ClO_4]_4$



Tetrakis-[2,4-di(3,5-dimethylpyrazol-1-yl)-6*H*-1,3,5-triazine]-tetrasilver(I) tetra-(hexafluoroantimonate)

$C_{52}H_{60}Ag_4F_{24}N_{28}Sb_4$

$[Ag_4(\mu\text{-}L^3)_4][SbF_6]_4$

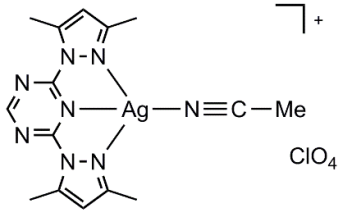


Tetrakis-[2,4-di(4,5,6,7-tetrahydroindazol-2-yl)-6*H*-1,3,5-triazine]-tetrasilver(I) tetraperchlorate

$C_{68}H_{76}Ag_4Cl_4N_{28}O_{16}$

$[Ag_4(\mu\text{-}L^4)_4][ClO_4]_4$

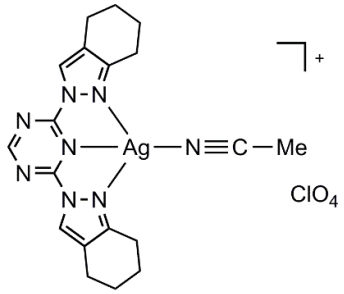
Complexes prepared during this study (continued)



[2,4-Di(3,5-dimethylpyrazol-1-yl)-6*H*-1,3,5-triazine]-(acetonitrile)silver(I) perchlorate

$C_{15}H_{18}AgClN_8O_4$

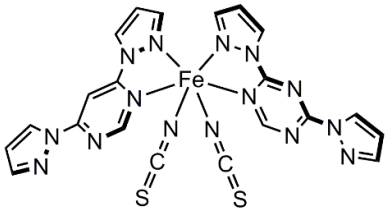
$[Ag(L^3)(NCMe)]ClO_4$



[2,4-di(4,5,6,7-tetrahydroindazol-2-yl)-6*H*-1,3,5-triazine]-(acetonitrile)silver(I) perchlorate

$C_{19}H_{22}AgClN_8O_4$

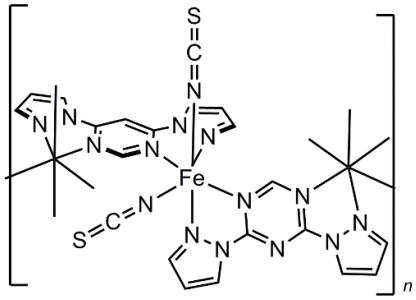
$[Ag(L^4)(NCMe)]ClO_4$



Bis-[4,6-di(pyrazol-1-yl)pyrimidine]-di[isothiocyanato]iron(II)

$C_{22}H_{16}FeN_{14}S_2$

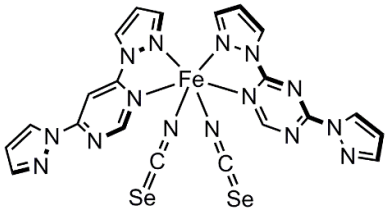
$[Fe(NCS)_2(L^5)_2]$



catena[4,6-di(pyrazol-1-yl)pyrimidine]-di[isothiocyanato]iron(II)

$C_{12}H_8FeN_8S_2$

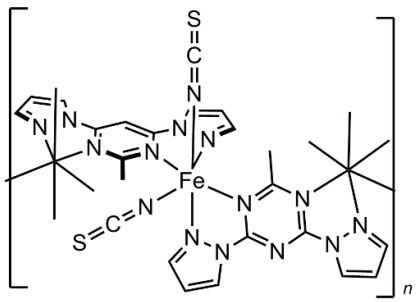
$[Fe(NCS)_2(\mu\text{-}L^5)]$



Bis-[4,6-di(pyrazol-1-yl)pyrimidine]-di[isoselenocyanato]iron(II)

$C_{22}H_{16}FeN_{14}Se_2$

$[Fe(NCSe)_2(L^5)_2]$

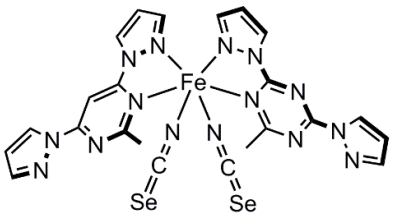


catena-[2-methyl-4,6-di(pyrazol-1-yl)pyrimidine]-di[isothiocyanato]iron(II)

$C_{13}H_{10}FeN_8S_2$

$[Fe(NCS)_2(\mu\text{-}L^6)]$

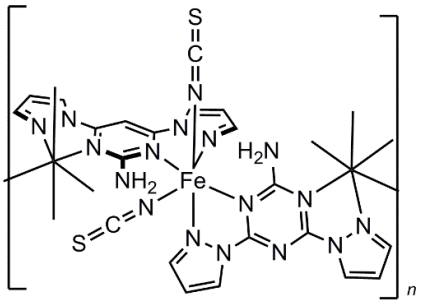
Complexes prepared during this study (continued)



Bis-[2-methyl4,6-di(pyrazol-1-yl)pyrimidine]-di[isoselenocyanato]iron(II)

$C_{24}H_{20}FeN_{14}Se_2$

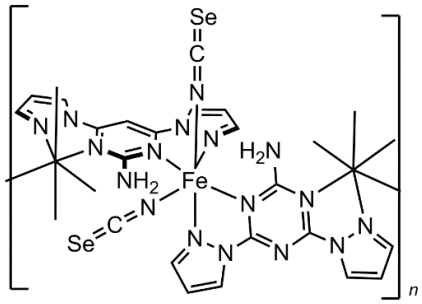
$[Fe(NCSe)_2(L^6)_2]$



catena-[2-amino-4,6-di(pyrazol-1-yl)pyrimidine]-di[isothiocyanato]iron(II)

$C_{12}H_9FeN_9S_2$

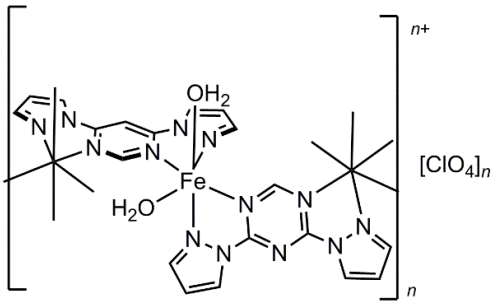
$[Fe(NCS)_2(\mu\text{-}L^7)]$



catena-[2-amino-4,6-di(pyrazol-1-yl)pyrimidine]-di[isoselenocyanato]iron(II)

$C_{12}H_9FeN_9Se_2$

$[Fe(NCSe)_2(\mu\text{-}L^7)]$



catena-[4,6-di(pyrazol-1-yl)pyrimidine]diaquairon(II) diperchlorate

$C_{10}H_{12}Cl_2FeN_6O_{10}$

$[Fe(OH_2)_2(\mu\text{-}L^5)][ClO_4]_2$